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Determination of the High-temperature Structures of Tugtupite using Synchrotron Radiation and Rietveld Refinements

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Beamline(s): X7B

The structural behaviour of tugtupite, (ideally $Na_8[Al_6Si_6O_{24}]Cl_2$), a member of the sodalite-group of minerals, was determined by using *in-situ* synchrotron radiation X-ray powder diffraction data (λ = 0.91997 Å) at room pressure and temperatures ranging from 38 to 985°C on heating. The sample was heated at a rate of about 9.5°C/min. and X-ray traces were collected at intervals of about 16°C. Eighteen structures in the temperature range were refined using the *GSAS* Rietveld refinement program. The variation of the volume with temperature is shown (Figure). Simultaneous differential scanning calorimetry (DSC) and thermogravimetry (TG) data were also obtained on tugtupite using a Netzsch STA 449C simultaneous TG-DSC instrument. Data were collected at a heating rate of 10°C/min. from 25 to 950°C. The peaks in the thermal curves are correlated with changes in the structural parameters. The unit-cell parameters for tugtupite increase quite smoothly and non-linearly to 985°C. In tugtupite, large displacement parameters occur for the Na and Cl atoms, and the Na - Cl bond expands with temperature. This forces the Na atoms toward the plane of the framework six-membered rings, which cause the framework tetrahedra to rotate. The framework TO_4 tetrahedra distorts with temperature, with the distortions following the sequence Si < Al < Be, which parallels the T - O bond strengths. This mechanism initially causes a high rate of expansion in tugtupite. If the Na atom reaches the plane of the six-membered ring, the expansion will be retarded, but tugtupite melts before this occurs. Tugtupite begins to lose NaCl at about 844°C (the total mass change to 950°C is -1.6%), and melts at about 1029°C.

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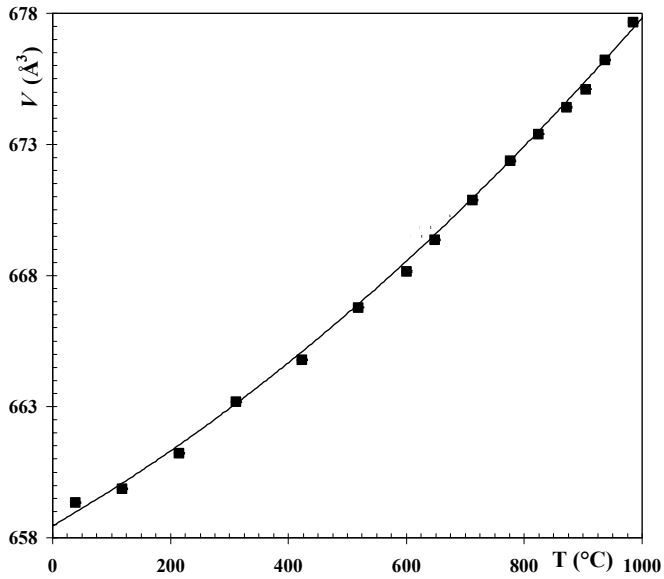

Figure: Variation of volume with temperature for tugtupite.